

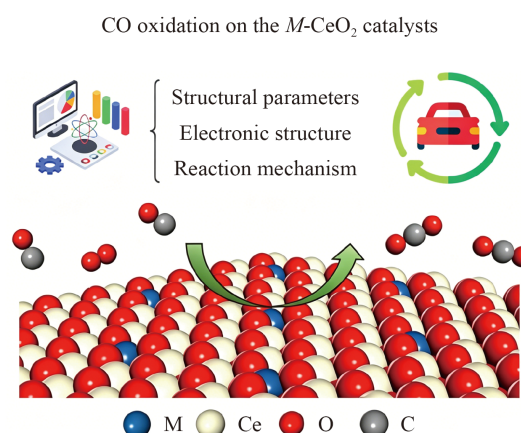
A database for CO oxidation over single-atom doped CeO₂ catalysts

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Abstract: Catalytic oxidation of CO, as a key reaction for reducing vehicle emissions, has been extensively studied. Introducing single atoms into ceria (CeO₂) is expected to combine the excellent oxygen storage/release capacity, reversible Ce⁴⁺/Ce³⁺ redox properties, and abundant surface defects of CeO₂, thereby further enhancing its catalytic performance in the low-temperature CO oxidation. However, existing first-principles calculation data remain scattered and systematic data for the single-atom doped CeO₂ catalysts (*M*-CeO₂) in the CO oxidation are lacking, which severely restricts the in-depth understanding of structure-performance relationships and reaction mechanisms concerning *M*-CeO₂. To address this gap, this study establishes a database covering a series of *M*-CeO₂ catalysts. Through DFT calculations, a multi-dimensional dataset was generated, which encompassed the model structures, elementary reaction energies, frequency analyses, density of states, bonding strengths and Bader charges. A rigorous quality control system was implemented for both computational parameters and output results to ensure the data integrity and reliability. This database, providing complete raw calculation files, offers a reliable foundation for exploring the catalytic performance, structure-performance relationships, and reaction mechanisms of *M*-CeO₂ catalysts in the low-temperature CO oxidation.

Key words: CeO₂; CO oxidation; database; first-principles calculation



Ceria (CeO₂), as a typical rare earth metal oxide, has been widely applied in the CO oxidation and other catalytic reactions due to its excellent oxygen storage/release capacity, reversible Ce⁴⁺/Ce³⁺ redox properties and abundant surface defect structures^[1–4]. Studies have indicated that the activity of CeO₂-based catalysts in CO oxidation can be significantly enhanced by adjusting the exposed crystal facets^[5–6], controlling the surface oxygen vacancy concentration^[7] and finely designing the local coordination environment of active sites^[8–9]. In recent years, transition metals in single-atom doped CeO₂ catalysts have exhibited excellent catalytic performance^[10–12]. The incorporation of single atoms into the CeO₂ lattice, where individual metal atoms substitute the surface Ce sites, is expected to retain the inherent redox properties of CeO₂ while tuning the electronic structure of active sites through the electronic and

geometric effects of the dopant atoms, providing new solutions for achieving efficient low-temperature CO oxidation^[13–16]. For example, theoretical calculations have shown that the Cu center in the Cu₁/CeO₂(111) single-atom catalyst (SAC) reversibly switches between Cu(I) and Cu(II) states; such a change is not random but precisely matches the reaction steps, thereby simultaneously optimizing reactant activation and product desorption, breaking the traditional “scaling relation” limitation in catalysis^[17]. However, systematic computational studies of single-atom doped CeO₂ catalysts (*M*-CeO₂) in CO oxidation remain relatively scattered, lacking unified data standards and high-throughput screening frameworks. Therefore, constructing a computational data system for the CeO₂-based SACs to systematically evaluate the stable configurations, electronic structures and CO oxidation

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reaction activities of different single metal atoms on the CeO₂ surface will not only help fill the gap in systematic theoretical data but also provide a reliable computational basis for revealing the catalytic mechanisms of single-atom doped CeO₂.

In this study, 20 transition metals elements spanning the 3d to 5d series are selected, including Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Y, Zr, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Pt and Au. The dopant atoms directly substitute surface Ce atoms of CeO₂(111), forming *M*-CeO₂ models with the *M*-O-Ce local coordination structures. This broad elemental selection aims to systematically investigate the regulatory effects of dopant atoms from different periods and with different electronic configurations on the catalytic performance of *M*-CeO₂(111) surface in the CO oxidation, providing a theoretical basis to reveal the intrinsic activity of dopant elements and rationally design efficient CeO₂-based catalysts for CO oxidation.

Hence, a specialized database was established for the

single-atom doped CeO₂ catalysts, which will provide a solid theoretical foundation for the screening and preparation of efficient catalysts in the CO oxidation. In addition, this database can also serve as an example of doped material databases, which may significantly promote the research progress in the ceria-based catalysts and related fields.

1 Data source

1.1 Dataset profile

This dataset, entitled “Database of CO oxidation over single-atom doped CeO₂ catalysts” (version V1.0; see Table 1), focuses on the performance and mechanisms of CO oxidation over CeO₂(111) and 20 *M*-CeO₂(111) catalysts. It also compiles the full structural data for these catalysts, along with the corresponding input and output files from the calculations.

Table 1 Basic information of the dataset

Data title	Database of CO oxidation over single-atom doped CeO ₂ catalysts
Data version	V1.0 (released in May 2026)
Software version	VASP5.4.4
Corresponding author	SONG Shaojia, ZHANG Riguang
Data authors	DU Kaiyue, SONG Shaojia, WANG Baojun, ZHANG Riguang
Time range	2024–2026
Data volume	191.00 GB, 10023 entries
Data format	*.zip
Data service system	CSTR: https://cstr.cn/31253.11.sciencedb.35455 . https://doi.org/10.57760/sciencedb.35455
Database composition	This database integrates comprehensive structural data and computational input/output files for pure CeO₂(111) and 20 <i>M</i>-CeO₂(111) catalysts. It is structured into five main components: (1) DFT calculation data of <i>M</i>-CeO₂ by VASP.zip (1.41 GB) contain the catalyst structures before and after optimization, and the adsorption configurations of reactants and products, along with the input and output files for transition state searches; (2) Frequency analysis data of <i>M</i>-CeO₂ by VASP.zip (118.99 MB) contain the input and output data from frequency calculations; (3) Bader charge data of <i>M</i>-CeO₂ by VASP.zip (5.56 GB) contain the input and output data from Bader charge analysis; (4) COHP data of <i>M</i>-CeO₂ by VASP.zip (150.30 GB) contain the input and output data from Crystal Orbital Hamilton Population (COHP) analysis; (5) DOS data of <i>M</i>-CeO₂ by VASP.zip (33.61 GB) contain the input and output data from density of states (DOS) calculations.
Citation format of data	DU K Y, SONG S J, WANG B J, et al. A database for CO oxidation over single-atom doped CeO₂ catalysts [J]. J Fuel Chem Technol, 2026, 54: 20260189. DU K Y, SONG S J, WANG B J, et al. Database of CO oxidation over single-atom doped CeO₂ catalysts [DS/OL]. V1. Science Data Bank, 2026[2026-06-30]. https://doi.org/10.57760/sciencedb.35455. DOI:10.57760/sciencedb.35455.

1.2 Structural models

The crystal structure of CeO₂ is obtained from the Materials Project database. A *p*(3×3) CeO₂(111) slab model containing 27 Ce atoms and 54 O atoms is employed. The

model consists of three O–Ce–O trilayers (nine atomic layers in total), where a vacuum layer of 15 Å is introduced perpendicular to the surface to eliminate periodic interactions^[18–19]. During optimization, the top six atomic layers and adsorbed species are allowed to relax, whereas the bottom three atomic layers are fixed at their bulk

positions. The database covers pure CeO₂ and a variety of metal-doped *M*-CeO₂ systems. Dopant metals (*M* = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Y, Zr, Mo, Ru, Rh, Pd, Ag, Ta, W, Re, Pt and Au) are introduced by substituting the surface Ce sites, resulting in a total of 20 structural models to systematically investigate the influence of different dopant elements on the catalytic performance.

Both pure CeO₂ and *M*-CeO₂ models are fully optimized to obtain the stable configurations, which are classified into five types based on their optimized structures (Figure 1). Type 1, Type 2-1, Type 2-2, Type 2-3 and Type 2-4, which are characterized by:

(1) Type 1: In the optimized catalyst, the metal atom substitutes the Ce site, and the catalyst structure retains the original CeO₂ configuration.

(2) Type 2-1: The metal atom is coordinated with two surface and three subsurface lattice oxygen atoms. The catalyst surface contains one two-coordinate oxygen.

(3) Type 2-2: The metal atom is coordinated with one surface and three subsurface lattice oxygen atoms. The catalyst surface contains two two-coordinate oxygen atoms.

(4) Type 2-3: The metal atom is coordinated with four subsurface lattice oxygen atoms. The catalyst surface contains three two-coordinate oxygen atoms.

(5) Type 2-4: Surface oxygen atoms undergo migration, resulting in the metal being coordinated with one one-coordinate oxygen, one surface oxygen atom and three subsurface oxygen atoms. The catalyst surface contains one two-coordinate oxygen.

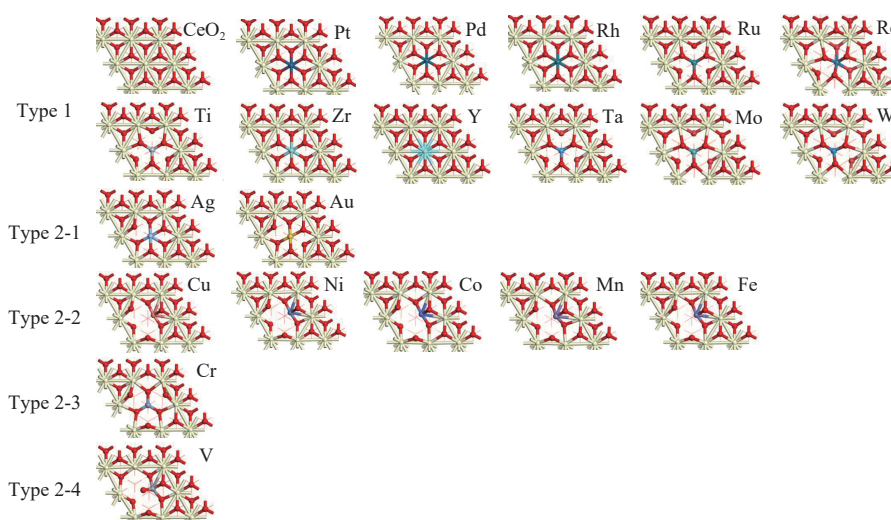


Fig. 1 Five types of coordination structures for *M*-CeO₂, namely Type 1, Type 2-1, Type 2-2, Type 2-3, Type 2-4

1.3 Computational details

All first-principles calculations are performed using the Vienna Ab-initio Simulation Package (VASP)^[20–21]. The interaction between ions and electrons is described by the projector augmented wave (PAW) method, with a plane-wave kinetic energy cutoff of 400 eV^[22–23]. The Brillouin zone is sampled only at the Γ point^[24]. The exchange-correlation effect is treated using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional^[25–26]. To accurately describe the interactions between electrons in the Ce 4*f* orbitals of *M*-CeO₂ catalysts, a Hubbard *U* correction ($U_{\text{eff}} = U - J$, where $J = 0$) is applied with a *U* value of 5.0 eV for the Ce 4*f* orbitals^[13,27]. For all structure optimizations, the force convergence criterion is 0.03 eV/Å and the energy convergence criterion is 1×10^{-6} eV. Transition state searches are carried out using the climbing-image nudged elastic band (CI-NEB) method and the dimer method^[28], with a final force convergence criterion of 0.05 eV/Å. Each transition state is verified by a single imaginary frequency.

Adsorption energies, reaction barriers, and elementary

reaction energies are all calculated based on the fully optimized stable structures. Free energy corrections under 423.15 K and 1 bar are applied using the VASPKIT tool^[29–30]. Electronic structure characterization methods, including bond strength (COHP), density of states (DOS), and Bader charge analysis, are employed to elucidate the regulation mechanism of dopant metals on the electronic properties of the CeO₂ surface^[31]. All input and output files are stored in a file system and the constructed database supports convenient retrieval, querying and usage functions.

1.4 Reaction mechanisms

Based on the kinetically calculated results, the most favorable pathway of CO oxidation is obtained: on the pure CeO₂, Type 1 (*M* = Ti, Y, Zr, Ru, Rh, Pd and Pt), Type 2-1, Type 2-2 and Type 2-4 catalysts, the CO oxidation reaction dominantly proceeds *via* two elementary steps: $\text{CO}^* + \text{O}_{\text{lat}} \rightarrow \text{CO}_2^*$ and $\text{CO}^* + \text{O}_2^* \rightarrow \text{CO}_2^* + \text{O}_{\text{lat}}$; on the Type 1 (*M* = Mo, Ta, W and Re) and Type 2-3 catalysts, it mainly proceeds *via* three elementary steps: $\text{CO}^* + \text{O}_{\text{lat}} \rightarrow \text{CO}_2^*$, $\text{CO}^* + \text{O}_{\text{lat}} \rightarrow \text{CO}_2^*$ and $\text{O}_2^* \rightarrow 2\text{O}_{\text{lat}}$.

1.5 Data content overview

This database, entitled “Database of CO oxidation reactions over single-atom doped CeO₂ catalysts”, systematically integrates complete structural data and computational input/output files for pure CeO₂(111) and 20 *M*-CeO₂(111) catalysts. It is structured into five main components:

(1) DFT calculation data package. The folder “DFT calculation data of *M*-CeO₂ by VASP.zip” contains complete DFT calculation results for the CO oxidation obtained using the VASP software. Taking Ti-CeO₂ as an example, the detailed data contents are described as follows: the “slab” folder contains the optimized and pre-optimized structural data for both the pristine surface and the single-oxygen-vacancy surface models, comprising 36 entries in total; the “ads” folder contains the adsorption configurations and associated optimized data for CO, O₂ and CO₂, comprising 108 entries in total; the “TS” folder contains the input files (including INCAR, POSCAR, etc.) and output files (including OUTCAR, CONTCAR, etc.) for the transition state search calculations of two elementary reaction steps, comprising 74 entries in total. The data volume under the Ti-CeO₂ folder amounts to 218 entries. The total size of “DFT calculation data of *M*-CeO₂ by VASP.zip” is 1.41 GB, with a total data volume of 4586 entries.

(2) Frequency analysis data package. The folder “Frequency analysis data of *M*-CeO₂ by VASP.zip” contains the input files (including INCAR, POSCAR, KPOINTS, etc.) and vibrational frequency data for the frequency analysis calculations of the initial state (IS), final state (FS) and transition state (TS) structures of elementary reactions, obtained using the VASP software. Taking Ti-CeO₂ as an example, the folder contains 110 data entries. The total size of “Frequency analysis data of *M*-CeO₂ by VASP.zip” is 118.99 MB, with a total data volume of 2557 entries.

(3) Bader charge analysis data package. The folder “Bader charge data of *M*-CeO₂ by VASP.zip” comprises the Bader charge dataset calculated using the VASP software. Taking Ti-CeO₂ as an example, the detailed data contents are described as follows: the “Ti-slab” folder contains the Bader charge calculation data for the total Ti-CeO₂ catalyst system, comprising 26 entries; the “Slab” folder contains the relevant data for the CeO₂ support system with the Ti atom removed, comprising 27 entries; the “Ti” folder contains the Bader charge calculation data for the isolated Ti atom, comprising 27 entries; the “CHGDIFF.vasp” file represents the charge density difference of the Ti-CeO₂ catalyst. The data volume under the Ti-CeO₂ folder amounts to 81 entries. The total size of “Bader charge data of *M*-CeO₂ by VASP.zip” is 5.56 GB, with a total data volume of 1700 entries.

(4) COHP bond strength analysis data package. The folder “COHP data of *M*-CeO₂ by VASP.zip” contains the input files (including INCAR, POSCAR, KPOINTS, etc.) and output files (including ICOHPLIST.lobster, etc.) for the calculations of bond length, bond energy and related

parameters of O–Ce and O–*M* bonds, obtained using the VASP software. Taking Ti-CeO₂ as an example, the folder contains 33 data entries. The total size of “COHP data of *M*-CeO₂ by VASP.zip” is 150.30 GB, with a total data volume of 697 entries.

(5) DOS analysis data package. The folder “DOS data of *M*-CeO₂ by VASP.zip” stores the complete input files (including INCAR, POSCAR, KPOINTS, etc.) and output files (including BAND_CENTER, PDOS_USER.dat, etc.) generated from the DOS calculations performed using the VASP software. Taking Ti-CeO₂ as an example, the folder contains 23 data entries. The total size of “DOS data of *M*-CeO₂ by VASP.zip” is 33.61 GB, with a total data volume of 483 entries.

The critical parameters for CeO₂ and *M*-CeO₂ are summarized in Table 2, which include the energy barrier of the rate-determining step, the *d*-band center of the dopant atom *M*, Bader charge and the O–Ce bond length. All data are organized and managed according to unified standards, providing comprehensive and reliable support for investigating *M*-CeO₂(111) in the catalytic oxidation of CO.

2 Data sample description

This database covers calculation parameters, structural information, software environment details and electronic properties for the single-atom doped CeO₂(111) catalysts in the CO oxidation. All calculation files are stored by catalyst type and organized in a unified, standardized directory structure. The Ti-CeO₂ system is used as an example to illustrate the file storage structure (Figures 2–6). All data files follow a consistent two-level folder naming convention: Level-1 folders are named by configuration type (Type 1, Type 2-1, Type 2-2, Type 2-3, Type 2-4), whereas Level-2 folders by single-atom metal type (e.g., CeO₂, Ti-CeO₂, Y-CeO₂, Zr-CeO₂ and Mo-CeO₂). The data contents are specified as follows:

(1) VASP calculation data (Figure 2). The folder “DFT calculation data of *M*-CeO₂ by VASP” contains calculation folders for 21 catalysts, covering the catalyst model geometry optimization and energy data (slab), reactant/intermediate/product adsorption structures and energy data, and TS search calculation results.

(2) Frequency analysis data (Figure 3). The folder “Frequency analysis data of *M*-CeO₂ by VASP” contains frequency analysis results for the elementary reactions on 21 stable catalyst structures, covering the IS, TS and FS structures for each reaction.

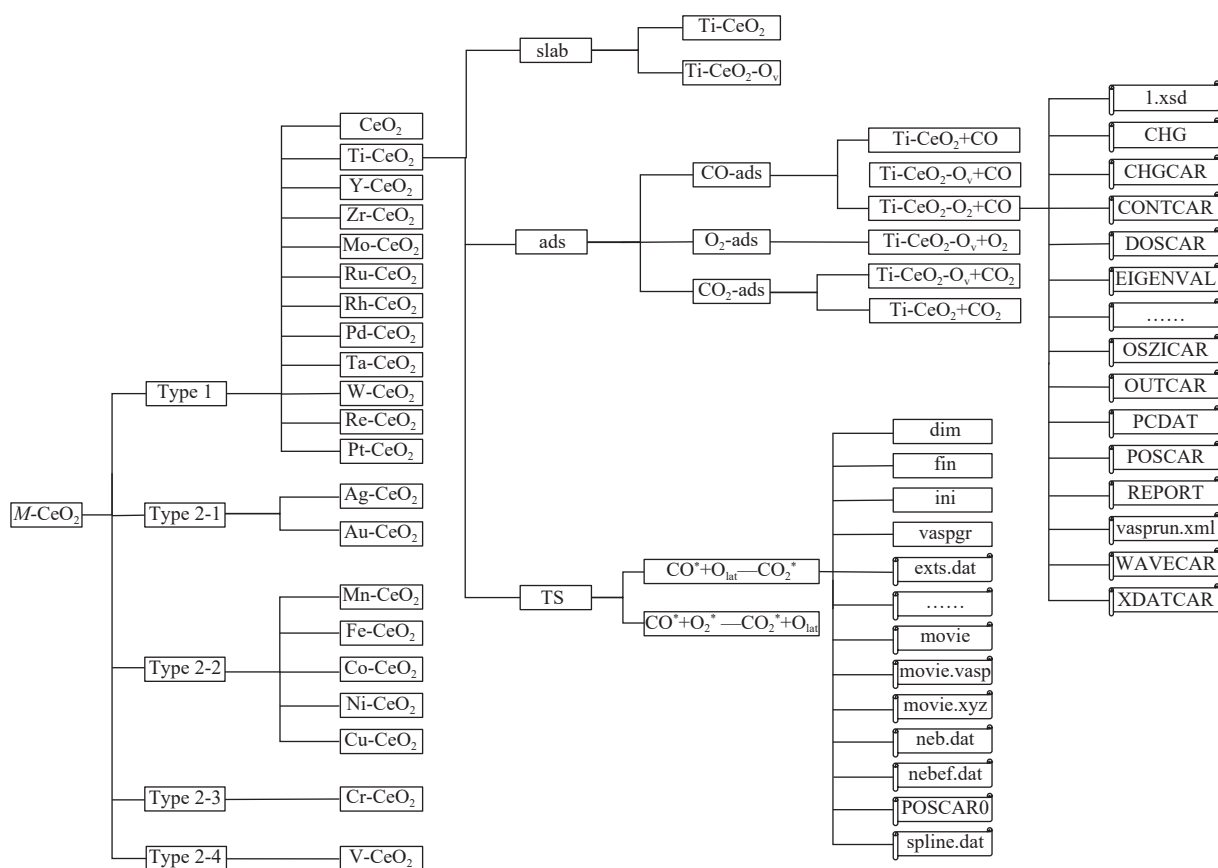
(3) Bader charge data (Figure 4). The folder “Bader charge data of *M*-CeO₂ by VASP” contains the Bader charge calculation and data processing results for 21 stable catalyst structures.

(4) COHP data (Figure 5). The folder “COHP data of *M*-CeO₂ by VASP” contains the COHP bond strength calculation and data processing results for 21 stable catalyst structures.

(5) DOS data (Figure 6). The folder “DOS data of *M*-CeO₂ by VASP” contains the DOS calculation and data processing results for 21 stable catalyst structures.

Table 2 Activation free energy of the rate-determining step, *d*-band center of the dopant atom *M*, Bader charge and O–Ce bond length for CeO₂ and *M*-CeO₂

Type	Catalyst	G_a/eV	<i>d</i> -band center/eV	Bader charge/e	O–Ce bond length/Å
Type 1	CeO ₂	0.92	−2.80	−2.40	2.34
	Ti-CeO ₂	0.57	−2.30	−2.18	2.59
	Y-CeO ₂	0.44	−2.67	−2.18	2.32
	Zr-CeO ₂	0.72	−2.80	−2.52	2.22
	Mo-CeO ₂	0.90	−5.85	−2.59	2.67
	Ru-CeO ₂	0.75	−2.38	−1.66	2.19
	Rh-CeO ₂	0.92	−1.67	−1.44	2.52
	Pd-CeO ₂	0.83	−1.86	−1.24	2.45
	Ta-CeO ₂	0.95	−5.37	−2.66	2.58
	W-CeO ₂	0.96	−6.18	−2.82	2.73
	Re-CeO ₂	1.10	−5.33	−2.57	2.80
	Pt-CeO ₂	0.77	−2.36	−1.34	2.46
Type 2-1	Ag-CeO ₂	0.62	−2.95	−1.13	2.28
	Au-CeO ₂	0.76	−2.83	−1.18	2.28
Type 2-2	Mn-CeO ₂	0.81	−1.00	−1.66	2.17
	Fe-CeO ₂	0.31	−1.84	−1.55	2.16
	Co-CeO ₂	0.51	−2.20	−1.34	2.15
	Ni-CeO ₂	0.74	−2.17	−1.21	2.17
	Cu-CeO ₂	0.71	−2.40	−1.13	2.21
Type 2-3	Cr-CeO ₂	0.36	−3.84	−1.80	2.19
Type 2-4	V-CeO ₂	0.83	−3.14	−2.10	2.18

Fig. 2 File storage directory structure in the DFT calculation data of *M*-CeO₂ by VASP.zip

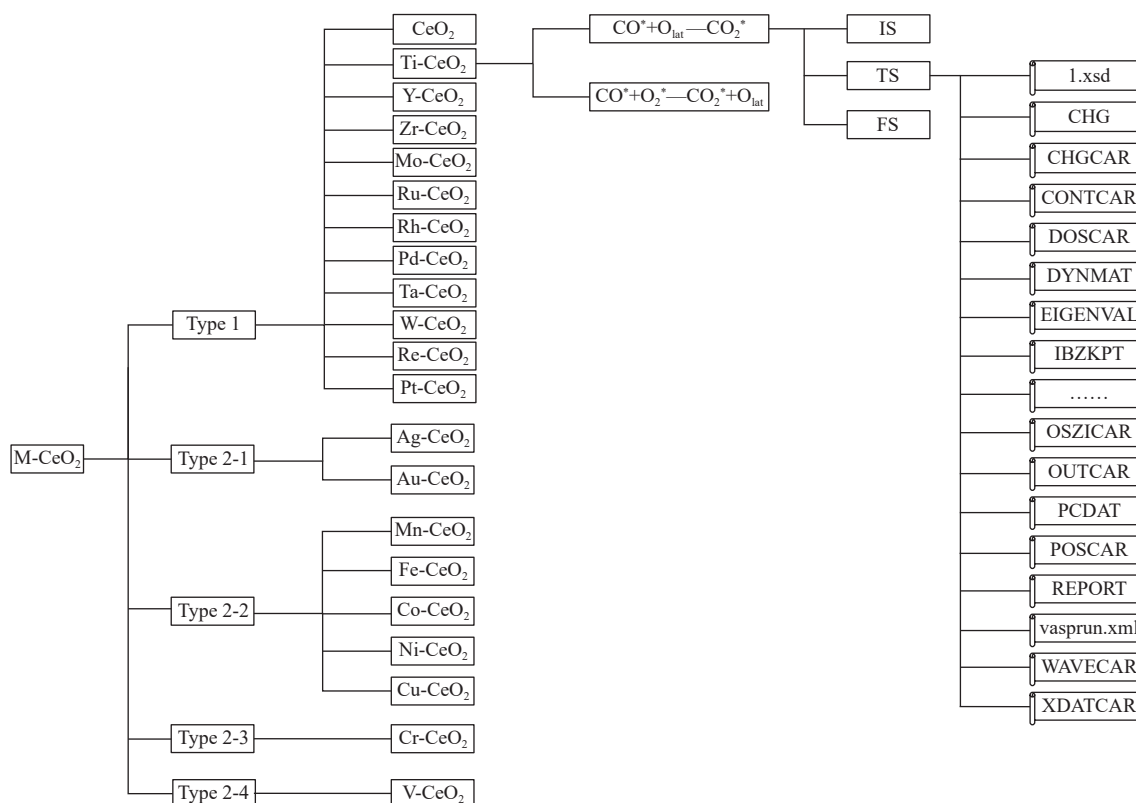


Fig. 3 File storage directory structure in the frequency analysis data of M -CeO₂ by VASP.zip

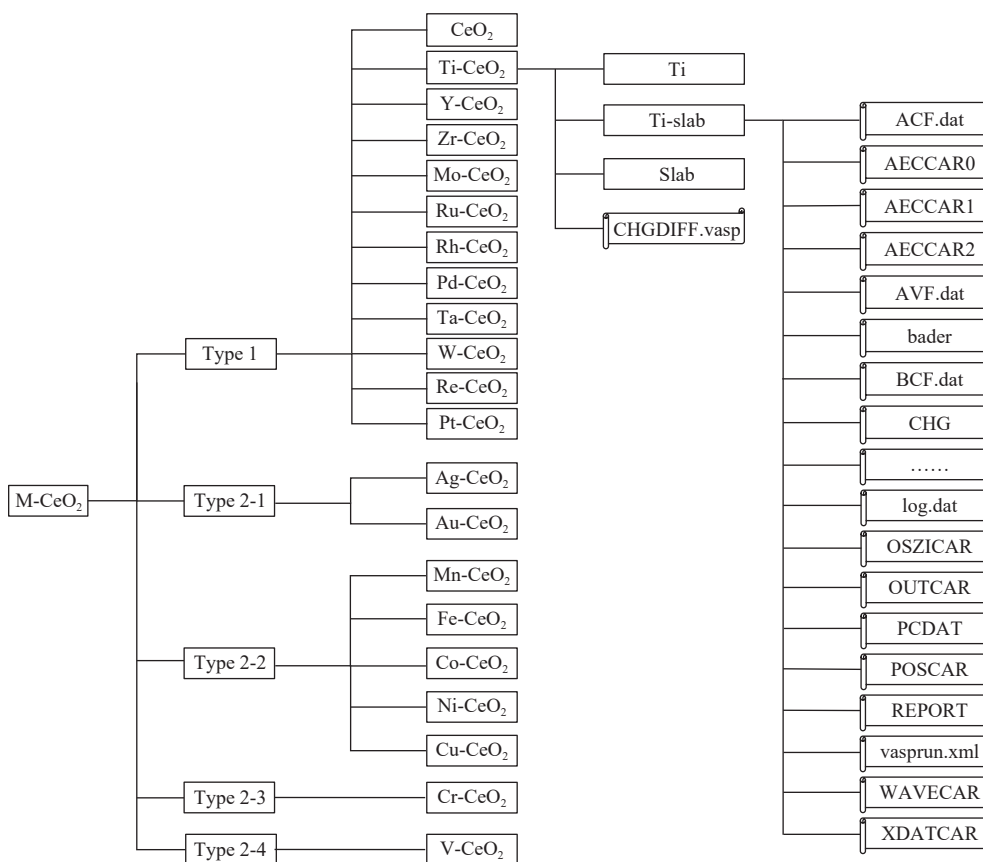


Fig. 4 File storage directory structure in the Bader charge data of M -CeO₂ by VASP.zip

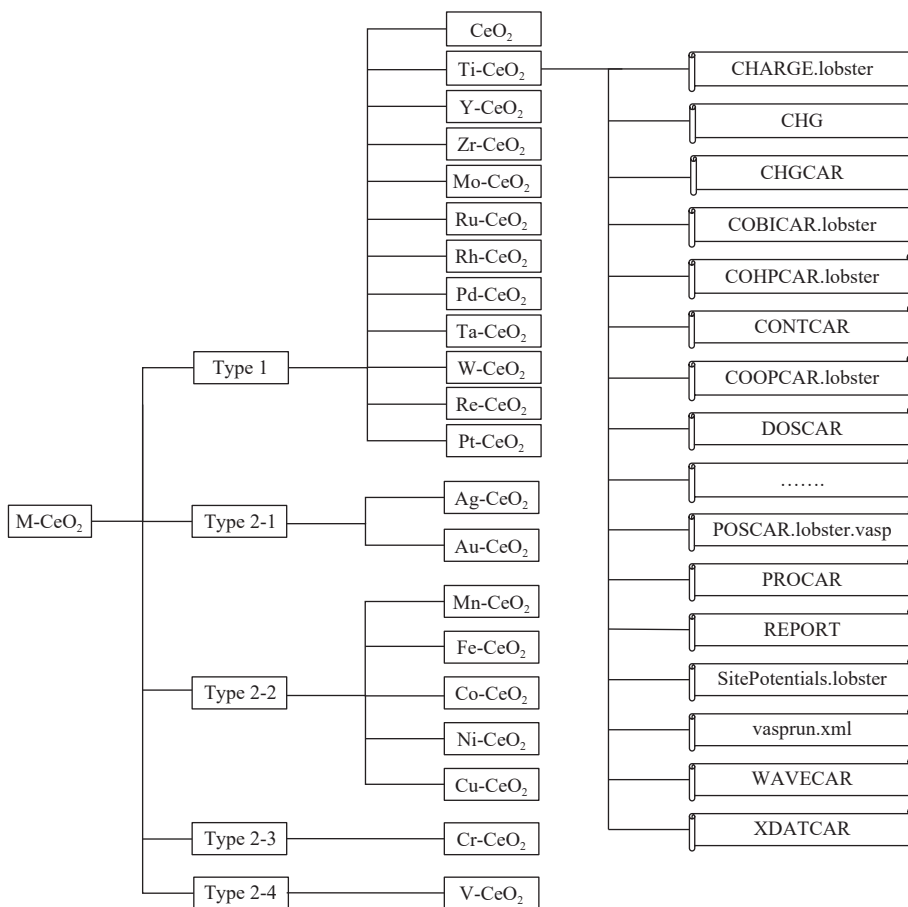


Fig. 5 File storage directory structure in the COHP data of $M\text{-CeO}_2$ by VASP.zip

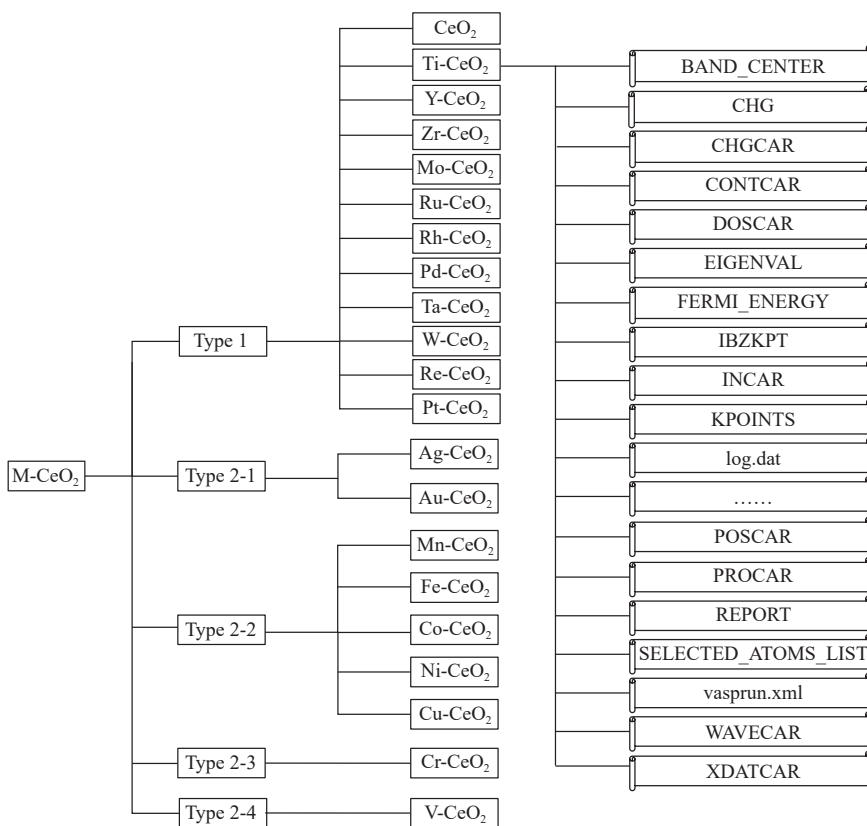


Fig. 6 File storage directory structure in the DOS data of $M\text{-CeO}_2$ by VASP.zip

3 Data quality control and evaluation

To ensure the stability and reliability of the calculated data, in the process of constructing the data set, this research has established strict convergence tests for key calculation parameters and results, ensuring that they all meet the strict convergence standards. All files have passed the convergence criteria specified in Section 3.1.

3.1 Convergence criterion

During calculations, strict convergence criteria must be adopted in the structural optimization and transition state search processes to ensure the reliability of calculation results. For VASP software, it can be confirmed by checking the output files (OUTCAR and OSZICAR) whether the electronic step (EDIFF) and ionic step (EDIFFG) are below the thresholds set in the input file (INCAR). In the OUTCAR file, the appearance of the sentence “reached required accuracy-stopping structural energy minimisation” indicates that the calculation has reached the convergence standard. Alternatively, one can check the last line of the OSZICAR file to estimate whether the energy change value (dE) is below the threshold; if so, the electronic step has converged.

Additionally, a systematic quality validation of the 10023 data entries in the database was performed to ensure that all structural optimization results meet $\text{EDIFF} \leq 1 \times 10^{-6}$ eV and $\text{EDIFFG} \leq 0.03$ eV/Å. In addition, all TS structures were verified by frequency analysis, showing exactly one imaginary frequency with the correct direction, while all IS and FS structures exhibit no imaginary frequencies in their frequency calculations. All computational results meet the data quality assessment criteria.

3.2 Handling of computational issues

In the DFT calculations, it is common to encounter situations where the computation cannot proceed smoothly, due to numerous causes including geometric structure problems, non-convergence of electronic steps, exhaustion of computing resources or insufficient memory and significant changes in magnetic moment. The corresponding solutions are presented as follows.

(1) Geometric structure problems: It is necessary to determine whether the calculation model is reasonable. If unreasonable, reconstruct a reasonable model and recalculate; if reasonable, calculate relative values based on the pristine model energy obtained from self-consistent calculations, thereby eliminating the influence of structural distortion on the calculation result accuracy.

(2) Non-convergence of electronic step: This can be resolved by adjusting calculation parameters such as MIXING and ALGO, or by gradually improving calculation accuracy through multiple relaxations.

(3) Exhausted computing resources or insufficient

memory: These issues can be addressed by increasing the number of convergence steps or expanding memory capacity.

(4) Significant changes in magnetic moment: This can be solved by performing the non-spin-polarized calculations to obtain stable charge density prior to the spin-polarized calculations.

4 Data value

This dataset systematically collects the complete input and output files for the DFT structural optimization, transition state searches and electronic property calculations (including DOS, COHP and Bader charge) of pristine $\text{CeO}_2(111)$ and 20 types of metal-doped $M\text{-CeO}_2(111)$ catalysts for the CO oxidation reaction. The initial computational configurations and output files provided in this dataset hold significant value for in-depth structural analysis and subsequent research. Users can directly access the raw data for result validation or data mining, enabling the reproduction of key reaction steps or the extraction of specific thermodynamic and kinetic parameters. Moreover, the comprehensive calculation files can serve as a foundation for extended investigations, facilitating advanced analyses such as barrier corrections and density of states interpretation.

For instance, researchers can directly invoke the frequency analysis data from the “Frequency analysis data of $M\text{-CeO}_2$ by VASP.zip” folder, and combine it with tools such as VASPKIT to perform free energy corrections under specific reaction temperatures, thereby accurately assessing the thermodynamic feasibility and kinetic barriers under reaction conditions. By retrieving the activation barriers and reaction energies of elementary reactions from the “DFT calculation data of $M\text{-CeO}_2$ by VASP.zip” folder, promising $M\text{-CeO}_2$ catalysts with high activity and superior catalytic performance potential for low-temperature CO oxidation can be rapidly screened, providing theoretical guidance for the experimental synthesis and effectively circumventing the limitations of the traditional trial-and-error approach for its long cycle times and high costs. Furthermore, by extracting the geometric structural features of stable catalyst configurations, the Bader charge transfer distribution in the active region, and electronic structure parameters such as bond lengths from the COHP database, researchers can systematically mine descriptors capable of accurately predicting the intrinsic activity of catalysts, thereby enabling efficient screening and rational design of catalysts.

5 Data usage guidelines and availability statement

The files in this database are available for direct download and are compatible with computational formats used by Materials Studio and VASP software. Due to copyright restrictions, pseudopotential files are not included

in this database.

All first-principles calculation data (with no external experimental data were used for comparison) presented in this paper—including structure optimization, frequency analyses, Bader charges analyses, COHP and DOS calculations for pure $\text{CeO}_2(111)$ and 20 $M\text{-CeO}_2(111)$ —are stored in the Science Data Bank (SDB) operated by the Computer Network Information Center, Chinese Academy of Sciences. The dataset is titled “Database of CO oxidation over single-atom doped CeO_2 catalysts” and is assigned with the following identifiers: Database DOI: <https://doi.org/10.57760/sciencedb.35455>; Database CSTR: <https://cstr.cn/31253.11.sciencedb.35455>. The dataset is accessible for download upon request *via* the platform and may be used for subsequent research.

Example 1 (Data retrieval). Researchers can retrieve the target data by following the directory structure illustrated in Figures 2–6. For example, to locate the structural and energetic data for the stable pristine surface configuration of the $\text{Pt-CeO}_2(111)$ system: First, select the folder “DFT calculation data of $M\text{-CeO}_2$ by VASP” within the compressed package; Second, following the directory hierarchy shown in Figure 2, navigate successively into the Pt-CeO_2 subfolder corresponding to the metal-doped system; Third, further locate the Pt-CeO_2 folder within the “slab” directory; Finally, invoke the “CONTCAR” file from this directory to obtain the optimized atomic coordinates and cell parameters and extract the total energy from the “OUTCAR” file.

Example 2 (Machine learning data support). Researchers can systematically invoke the geometric structural descriptors, energy data, Bader charge transfer data, and relevant feature values from the COHP and DOS folders for the 20 types of $M\text{-CeO}_2$ catalysts in the database, serving as the input feature set for machine learning models. Based on these multi-dimensional data, one can not only analyze the microscopic origins of coordination environment differences among various $M\text{-CeO}_2$ catalysts, revealing the intrinsic correlations among metal dopant type, local coordination structure, and electronic properties, but also screen and construct a descriptor system capable of accurately predicting the catalytic activity for low-temperature CO oxidation, such as intrinsic parameters including the Bader charge of the metal center, the d -band center, or specific bond lengths. Furthermore, by leveraging the trained machine learning model, rapid prediction and preliminary screening of the catalytic performance of other single-atom-modified CeO_2 catalysts can be achieved, providing a data-driven theoretical support for the rational design of novel catalysts of high-efficiency and effectively shortening the experimental exploration cycle.

6 Conclusions

To address the problems that systematic computation studies of $M\text{-CeO}_2$ in the low-temperature CO oxidation are

relatively scattered and lack unified data standards, this study employs first-principles calculations to construct a database for the $M\text{-CeO}_2$ single-atom catalysts, systematically revealing the differences in catalytic performance of single-atom types and doping structures in various elementary reaction steps. This database can not only be used to evaluate the catalytic activity in the CO oxidation by referencing reaction energies, but also to establish structure-performance relationships among “dopant metal—electronic properties—catalytic activity” by correlating reaction energies with electronic properties. With the aid of COHP, DOS and Bader charge analyses, the mechanisms underlying performance differences are explained at the electronic level, providing theoretical basis for the rational design of efficient in the catalysts CO oxidation. This work demonstrates the feasibility of generating well-structured, information-complete and mechanism-explicit domain-specific datasets through large-scale calculations. Furthermore, this scientific database will be continuously enriched and optimized through experimental comparison and validation, which helps to promote the research of low-temperature catalytic CO oxidation toward a new data-driven paradigm.

Declaration of Competing Interest

The authors declare no conflict of interest.

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单原子掺杂二氧化铈催化剂上一氧化碳氧化反应的数据库

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摘要: 一氧化碳(CO)催化氧化是汽车尾气减排的关键反应之一, 已受到研究人员的广泛关注。将金属单原子引入二氧化铈(CeO_2)载体, 有望借助 CeO_2 优异的储氧/释氧能力、可逆的 $\text{Ce}^{4+}/\text{Ce}^{3+}$ 氧化还原特性及丰富的表面缺陷, 进一步提升其低温 CO 氧化的催化性能。目前, 基于第一性原理的计算数据较为分散, 缺乏针对单原子掺杂 CeO_2 催化剂($M\text{-CeO}_2$)在 CO 氧化过程中系统性的理论数据, 这严重制约了对该类催化剂构效关系和反应机理的深入认识。针对这一现状, 本研究构建了涵盖多种过渡金属元素的 $M\text{-CeO}_2$ 催化剂数据库。通过 DFT 计算, 生成了包含模型结构、基元反应能量、频率分析、态密度、成键强度和 Bader 电荷等多维度信息的数据集, 并在计算参数设置与输出结果两方面建立了严格的质量控制体系, 以保障数据的完整性与可靠性。该数据库同时提供完整的原始计算文件, 为研究 $M\text{-CeO}_2$ 催化剂在低温 CO 催化氧化中的性能、构效关系及反应机理提供了可靠的数据基础。

关键词: 二氧化铈; 一氧化碳氧化; 数据库; 第一性原理计算

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